UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

SUBJECT: Product Chemistry Review of Technical Bromadiolone (EPA ID No. 12455-TN)

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SEP 5 1991

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APPLICANT: Bell Laboratories, Inc.

EPA ID NO: 12455-TN

MRID NOS: 417170-00, 417170-01, 417170-02, 417170-03

CAS NO: 28772-56-7

PESTICIDE CHEMICAL CODE(PCC): 112001

CHEMICAL NAME: 3-[3-(4'-Bromobiphenyl-4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxycoumarin

PRODUCT NAME: Bromadiolone

USE: Rodenticide

INTRODUCTION

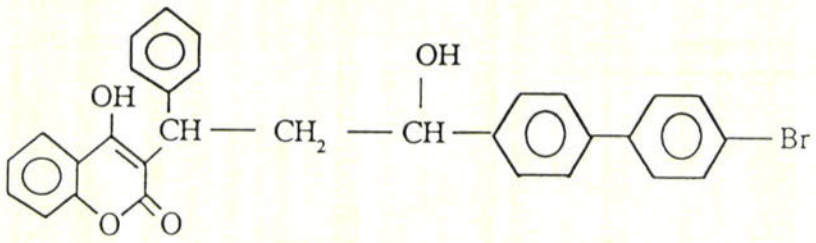
Bell Laboratories, Inc. requests the registration of the manufacturing-use product (MP) Technical Bromadiolone which contains the active ingredient (ai) Bromadiolone. The applicant contends that the product is substantially similar to the registered product EPA Reg. No. 7173-174. All product chemistry requirements for the MP as described in CFR 158.150 must be fulfilled for full registration.

PRODUCT IDENTITY AND COMPOSITION (MRID 417170-01)

61-1: Product Identity and Disclosure of Ingredients

Bromadiolone is the active ingredient (ai) in the MP produced by Bell Laboratories, Inc. Bromadiolone is:

3-[3-(4'-bromobiphenyl-4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxycoumarin (IUPAC)



Empirical Formula: $C_{30}H_{23}BrO_4$

Molecular Weight: 527.4

OTHER NAMES

3-[3-(4'-bromo[1,1'-biphenyl]-4-yl)-3-hydroxy-1-phenylpropyl-4-hydroxy-2H-1-benzoyran-2-one

3-[alpha-[p-(p-bromophenyl)-beta-hydroxyphenethyl]benzyl-4-hydroxycoumarin]

The composition of the MP is contained in the Confidential Statement of Formula (CSF, EPA Form 8570-4) and is discussed in Confidential Appendix B.

The data satisfy the requirements of 40 CFR 158.155. No additional data are needed.

61-2: Beginning Materials and Manufacturing Process

See Confidential Appendix A for a discussion of the beginning materials and the manufacturing process.

The data satisfy the requirements of 40 CFR 158.160-162. No additional data are needed.

61-3: Discussion of the Formation of Impurities

See Confidential Appendix A for a discussion of the formation of impurities.

The data satisfy the requirements of 40 CFR 158.167 for the MP. No additional data are needed.

ANALYSIS AND CERTIFICATION OF PRODUCT INGREDIENTS (MRID 417170-02)

62-1: Preliminary Analysis

Samples from five batches of the MP were examined for the ai bromadiolone and its impurities. For a discussion of the results and the analytical methods used, see Confidential Appendix B.

The submitted data satisfy the requirements of 40 CFR 158.170. No additional data are needed.

62-2: Certified Limits

The certified limits are contained in the CSF and are discussed in Confidential Appendix B.

The submitted data do not satisfy the requirements of 40 CFR 158.175 for the MP Technical Bromadiolone. The following

information should be submitted: (1) A revised CSF which contains the identification of each isomer of the active ingredient mixture. The nominal and certified limits for each component should also be included; (2) A discussion on whether both isomers contain pesticidal activity.

62-3: Enforcement Analytical Methods

The analytical methods submitted for enforcement are discussed in Confidential Appendix B.

An adequate analytical method is submitted for enforcement purposes for the active ingredients. The submitted information satisfy the requirements for 40 CFR 158.180.

PHYSICAL AND CHEMICAL CHARACTERISTICS (MRID 417170-03)

The physicochemical properties of Technical Bromadiolone (MP) are summarized below.

guidelines Reference Number (GRN)	Property	Description
63-2	Color	White
63-3	Physical State	Powder
63-4	Odor	None
63-5	Melting Point	205 - 210 °C
63-6	Boiling Point	Not Applicable (N/A)
63-7	Bulk Density	0.33 g/ml
63-8	Solubility	Solvent / Quantity Water / 6.1 ppm Hexane / <0.001g/100ml Ethanol / 0.5g/100ml Diethyl Ether / 0.017g/100ml Acetone / 1.15g/100ml
63-9	Vapor Pressure	N/A (m.p.>30 °C)
63-10	Dissociation Constant	5.73
63-11	Octanol/Water Partition Coefficient	1.44
63-12	pH	4.48 (1% soln. in 75:25 Dioxane:Water)
63-13	Heat Stability	Stable*
63-14	Oxidizing or Reducing Action	N/A
63-15	Flammability	N/A
63-16	Explodability	Non-Explosive
63-17	Storage Stability	Study is underway
63-18	Viscosity	N/A
63-19	Miscibility	N/A
63-20	Corrosion Characteristics	Non-reactive & non-corrosive to metal, plastic & paper

63-21: Dielectric Breakdown Voltage N/A

(*) The information on Stability (GRN 63-13) should include discussion of the sensitivity of the active ingredient to metal ions and metal and the sensitivity of the active ingredient to sunlight.

SUMMARY OF DEFICIENCIES

The Product Chemistry data requirements for the MP, Technical Bromadiolone, have not been satisfied. The following information is needed.

62-2: Certified Limits

A revised CSF which contains the identification and the nominal and certified limits for each isomer of the active ingredient mixture should be submitted. Additionally, a discussion should be submitted on whether one or both isomers possess pesticidal activity and/or are active toward biological systems.

63-13: Stability

A discussion of the sensitivity of the active ingredient to metal ions and metal and the sensitivity of the active ingredient to sunlight should be submitted.

CONCLUSION ON SUBSTANTIAL SIMILARITY

(See Data Review Instructions, Bean Sheet dated 5/21/91)

PCRS/RSB is not able to determine if the Bell Laboratories products are substantially similar to the registered product (EPA Reg. No. 7173-174) due to the deficiencies noted in item 62-2 above. When these deficiencies are resolved, then a comparison of the products may be made to determine if substantial similarity exists.

ATTACHMENTS: Confidential Appendices A and B.

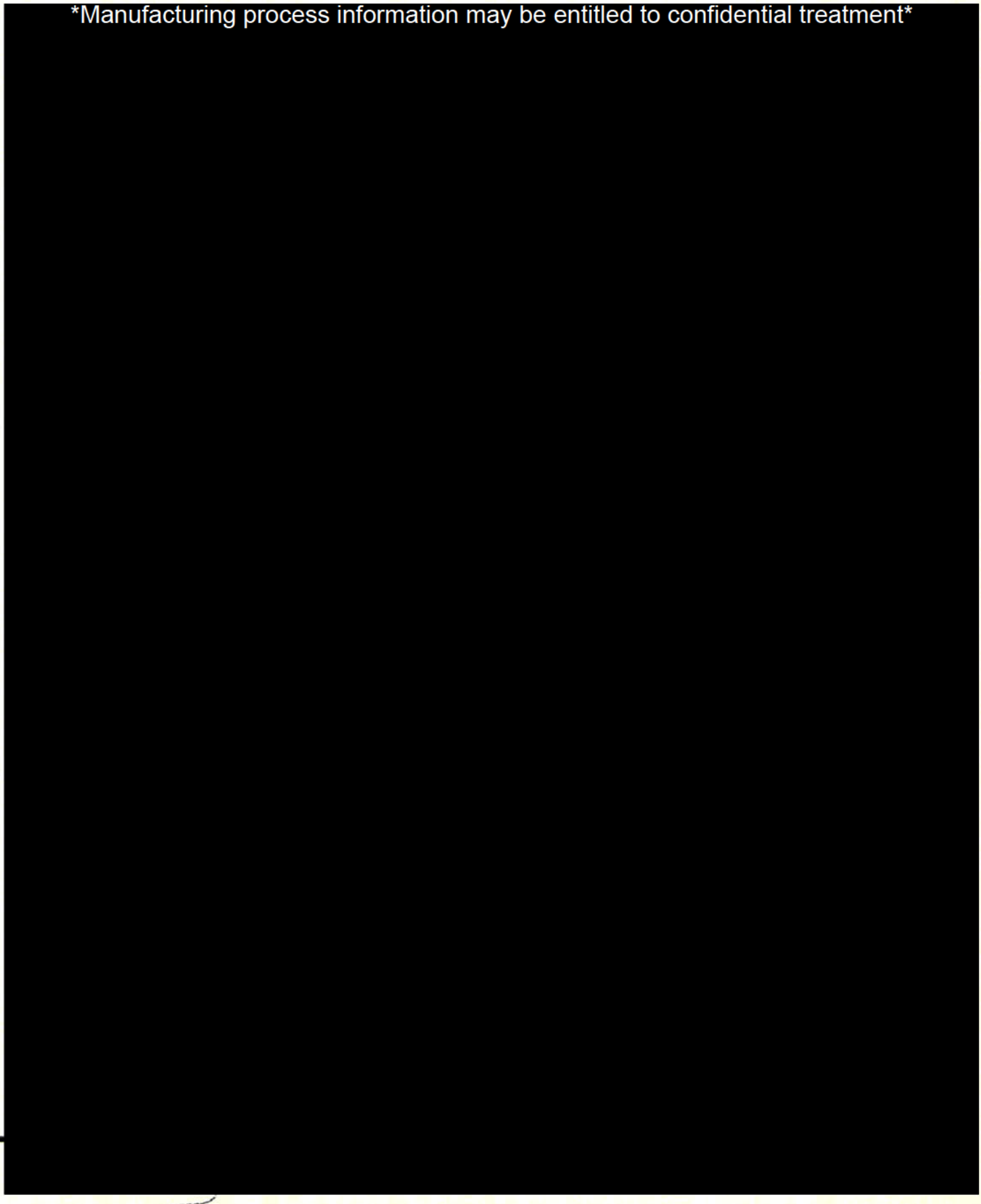
CONFIDENTIAL APPENDIX A

Manufacturing process information may be entitled to confidential treatment

[redacted]

Figure 1

Manufacturing process information may be entitled to confidential treatment



CONFIDENTIAL APPENDIX A

Manufacturing process information may be entitled to confidential treatment

[redacted]

CONFIDENTIAL APPENDIX B

Manufacturing process information may be entitled to confidential treatment

[redacted]

CONFIDENTIAL APPENDIX B

Manufacturing process information may be entitled to confidential treatment

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CONFIDENTIAL APPENDIX B

Manufacturing process information may be entitled to confidential treatment

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